Solvent Effects on Protein Motion and Protein Effects on Solvent Motion

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Abstract

Proteins present rough, chemically heterogeneous, and dynamic surfaces to their solvent, which for most proteins is primarily aqueous[1]. Roughly a monolayer of water, the so-called hydration water is perturbed structurally and dynamically by interaction with the protein[2]. We will present results from several experimental and molecular dynamics simulation studies[2, 3, 4, 5] that illustrate the anomalous properties of hydration water, and demonstrate that hydration water is crucial for protein function. We will also discuss the coupling of functionally important protein motions to water dynamics[6], as well as how this coupling can be tuned by changing the solvent composition[7].

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